U Kell, Douglas B.; Goodacre, Royston; Neal, Mark J.
S Institute of Biological Sciences, University of Wales, Aberystwyth, SY23 3DA, UK
O Proceedings of the ERDEC Scientific Conference on Chemical and Biological Defense Research, Aberdeen Proving Ground, Md., Nov. 14-17, 1995 (1996), Meeting Date 1995, 183-189. Editor(s): Berg, Dorothy A. Publisher: National Technical Information Service, Springfield, Va.
CODEN: 64OYA8
T Conference
LA English

> s specimen? and l15
264666 SPECIMEN?
16 1 SPECIMEN? AND L15

> d

L16 ANSWER 1 OF 1 CA COPYRIGHT 2004 ACS on STN
AN 128:50824 CA
I Application of laser microprobe inductively coupled plasma mass spectrometry for trace metal **fingerprinting** of native gold
AU Chen, Zhongxing; Doherty, Will; Gregoire, D. Conrad; Harris, Don
CS Dept. of Geology, Mineral Resources Division, University of Windsor, Windsor, ON, N9B 3P4, Can.
O Current Research - Geological Survey of Canada (1997), (1997-D), 57-62
CODEN: CRGCED; ISSN: 0704-2884
PB Geological Survey of Canada
DT Journal
LA English
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

> d ab

L16 ANSWER 1 OF 1 CA COPYRIGHT 2004 ACS on STN
AB Major, minor, and trace elements in 60 native Au samples from across Canada were analyzed directly by laser ablation microprobe inductively coupled plasma-mass spectrometry (LAM-ICP-MS). Diams. of laser ablation craters ranged from 100 to 150 μm defining the smallest sample size determinable. The Au signal was used as an internal standard to correct for differences in ablation yields, matrix effects and signal **drift** during anal. Anal. results obtained over a period of seven months for the synthetic Au alloy standard 501 demonstrated the long-term reproducibility of the method. The elemental signatures obtained from individual **specimens** have proven to be unique and reproducible, yielding data that can be used for matching "unknowns" with their source location.

> d l4 4

L4 ANSWER 4 OF 4 CA COPYRIGHT 2004 ACS on STN
AN 124:81135 CA
I Correction of Mass Spectral **Drift** Using Artificial Neural Networks
AU **Goodacre, Royston**; Kell, Douglas B.
CS Institute of Biological Sciences, University of Wales, Aberystwyth/Dyfed, SY23 3DA, UK
O Analytical Chemistry (1996), 68(2), 271-80
CODEN: ANCHAM; ISSN: 0003-2700
PB American Chemical Society
DT Journal
LA English

> log y
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

ULL ESTIMATED COST	122.93	124.28
ISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
A SUBSCRIBER PRICE	-7.92	-7.92

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                  resulting in a closer connection to BABS
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                  fields
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                  Patent Office Classifications
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                  (Version 7.01 for Windows) now available
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                  status data from INPADOC
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 NEWS 12  SEP 27  STANDARDS will no longer be available on STN
 NEWS 13  SEP 27  SWETSCAN will no longer be available on STN
 NEWS 14  OCT 28  KOREAPAT now available on STN

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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FILE 'HOME' ENTERED AT 14:52:08 ON 15 NOV 2004

=> file medline
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004

 FILE LAST UPDATED: 13 NOV 2004 (20041113/UP).  FILE COVERS 1950 TO DATE.

 On February 29, 2004, the 2004 MeSH terms were loaded.  See HELP RLOAD
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for details.

OLDMEDLINE now back to 1950.

MEDLINE thesauri in the /CN, /CT, and /MN fields incorporate the
MeSH 2004 vocabulary. See http://www.nlm.nih.gov/mesh/ and
http://www.nlm.nih.gov/pubs/techbull/nd03/nd03_mesh.html for a
description of changes.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> e goodacre/au
E1            1     GOODA K/AU
E2            2     GOODA S A/AU
E3            0 --> GOODACRE/AU
E4           22     GOODACRE A/AU
E5            6     GOODACRE A M/AU
E6            1     GOODACRE ANGELA/AU
E7           10     GOODACRE B/AU
E8            2     GOODACRE B B/AU
E9            1     GOODACRE B C/AU
E10          20     GOODACRE B W/AU
E11           1     GOODACRE BRIAN/AU
E12           4     GOODACRE BRIAN W/AU

=> e goodacre royston/au
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E2           17     GOODACRE R L/AU
E3           22 --> GOODACRE ROYSTON/AU
E4           24     GOODACRE S/AU
E5            1     GOODACRE S C/AU
E6            2     GOODACRE S H/AU
E7            2     GOODACRE S L/AU
E8           11     GOODACRE S W/AU
E9            1     GOODACRE SARA L/AU
E10           7     GOODACRE STEVE/AU
E11           1     GOODACRE STEVE W/AU
E12          14     GOODACRE T/AU

=> s e3
L1           22 "GOODACRE ROYSTON"/AU

=> d ti 1-22

L1   ANSWER 1 OF 22     MEDLINE on STN
TI   Differentiation of Micromonospora Isolates from a Coastal Sediment in
     Wales on the Basis of Fourier Transform Infrared Spectroscopy, 16S rRNA
     Sequence Analysis, and the Amplified Fragment Length Polymorphism
     Technique.

L1   ANSWER 2 OF 22     MEDLINE on STN
TI   Comparison of diffuse-reflectance absorbance and attenuated total
     reflectance FT-IR for the discrimination of bacteria.

L1   ANSWER 3 OF 22     MEDLINE on STN
TI   Surface-enhanced Raman spectroscopy for bacterial discrimination utilizing
     a scanning electron microscope with a Raman spectroscopy interface.

L1   ANSWER 4 OF 22     MEDLINE on STN
TI   Selective detection of proteins in mixtures using electrospray ionization
     mass spectrometry: influence of instrumental settings and implications for
     proteomics.

L1   ANSWER 5 OF 22     MEDLINE on STN
TI   Metabolomics by numbers: acquiring and understanding global metabolite
     data.

L1   ANSWER 6 OF 22     MEDLINE on STN
```

I Whole-organism fingerprinting of the genus Carnobacterium using Fourier transform infrared spectroscopy (FT-IR).

1 ANSWER 7 OF 22 MEDLINE on STN
I Ultra-violet resonance Raman spectroscopy for the rapid discrimination of urinary tract infection bacteria.

1 ANSWER 8 OF 22 MEDLINE on STN
I Metabolic profiling: pathways in discovery.

1 ANSWER 9 OF 22 MEDLINE on STN
I Characterization of microorganisms using UV resonance Raman spectroscopy and chemometrics.

1 ANSWER 10 OF 22 MEDLINE on STN
I Discrimination of bacteria using surface-enhanced Raman spectroscopy.

1 ANSWER 11 OF 22 MEDLINE on STN
I Application of high-throughput Fourier-transform infrared spectroscopy in toxicology studies: contribution to a study on the development of an animal model for idiosyncratic toxicity.

1 ANSWER 12 OF 22 MEDLINE on STN
I Explanatory optimization of protein mass spectrometry via genetic search.

1 ANSWER 13 OF 22 MEDLINE on STN
I Rapid quantitative assessment of the adulteration of virgin olive oils with hazelnut oils using Raman spectroscopy and chemometrics.

1 ANSWER 14 OF 22 MEDLINE on STN
I Investigating plant-plant interference by metabolic fingerprinting.

1 ANSWER 15 OF 22 MEDLINE on STN
I Metabolic fingerprinting of salt-stressed tomatoes.

1 ANSWER 16 OF 22 MEDLINE on STN
I Chemometric discrimination of unfractionated plant extracts analyzed by electrospray mass spectrometry.

1 ANSWER 17 OF 22 MEDLINE on STN
I Metabolic profiling using direct infusion electrospray ionisation mass spectrometry for the characterisation of olive oils.

1 ANSWER 18 OF 22 MEDLINE on STN
I Fluorescent amplified fragment length polymorphism probabilistic database for identification of bacterial isolates from urinary tract infections.

1 ANSWER 19 OF 22 MEDLINE on STN
I Monitoring of complex industrial bioprocesses for metabolite concentrations using modern spectroscopies and machine learning: application to gibberellic acid production.

1 ANSWER 20 OF 22 MEDLINE on STN
I Sample preparation in matrix-assisted laser desorption/ionization mass spectrometry of whole bacterial cells and the detection of high mass (>20 kDa) proteins.

1 ANSWER 21 OF 22 MEDLINE on STN
I Rapid and quantitative detection of the microbial spoilage of meat by fourier transform infrared spectroscopy and machine learning.

1 ANSWER 22 OF 22 MEDLINE on STN
I Flow-injection electrospray ionization mass spectrometry of crude cell extracts for high-throughput bacterial identification.

> s l1 and drift
5370 DRIFT
2 0 L1 AND DRIFT

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> file ca
OST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                        ENTRY     SESSION
ULL ESTIMATED COST                                       1.14        1.35

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ILE LAST UPDATED: 11 Nov 2004  (20041111/ED)

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> e goodacre r/au
1            7     GOODACRE JOHN A/AU
2            1     GOODACRE PAUL R/AU
3           19 --> GOODACRE R/AU
4            1     GOODACRE ROBERT/AU
5            1     GOODACRE ROBERT L/AU
6           86     GOODACRE ROYSTON/AU
7            1     GOODACRE S/AU
8            1     GOODACRE SARA/AU
9            1     GOODACRE SARA L/AU
10           2     GOODACRE SIMON/AU
11           3     GOODACRE SIMON C/AU
12          21     GOODACRE SIMON CHARLES/AU

> s e6
3           86 "GOODACRE ROYSTON"/AU

> s drift and l3
        34318 DRIFT
4           4 DRIFT AND L3

> d ti 1-4

4   ANSWER 1 OF 4  CA  COPYRIGHT 2004 ACS on STN
I   On mass spectrometer instrument standardization and interlaboratory
    calibration transfer using neural networks

4   ANSWER 2 OF 4  CA  COPYRIGHT 2004 ACS on STN
I   Rapid analysis of multiple determinands using pyrolysis mass spectrometry
    and supervised learning with artificial neural networks - principles and
    applications

4   ANSWER 3 OF 4  CA  COPYRIGHT 2004 ACS on STN
I   Analyzing a sample by using a neural network to correct for measurement
    drift

4   ANSWER 4 OF 4  CA  COPYRIGHT 2004 ACS on STN
I   Correction of Mass Spectral Drift Using Artificial Neural
    Networks
```

> d ab 1-4

L4 ANSWER 1 OF 4 CA COPYRIGHT 2004 ACS on STN
AB For pyrolysis mass spectrometry (PyMS) to be exploited in areas such as the routine identification of microorganisms, for quantifying determinants in biol. and biotechnol. systems, and in the production of useful mass spectral libraries, it is paramount that newly acquired spectra be comparable to those previously collected and held in a central reference laboratory Artificial neural networks (ANNs) and other multivariate calibration models have been used to relate mass spectra to the biol. features of interest. However, calibration models developed on one mass spectrometer cannot be used with spectra collected on a second instrument, because of the differences between the instrumental responses of both instruments. We report here that an ANN-based **drift** correction procedure can be implemented so that newly acquired spectra can be used to challenge models constructed using mass spectra collected on different instruments. Calibration samples were run on three different PyMS machines, and ANNs set up in which the inputs were the 150 machine 'a' calibration masses and the outputs were the 150 calibration masses from the machine 'b' spectra. Such associative neural networks could thus be used as signal-processing elements to effect the transformation of data acquired on one machine to those which would have been acquired on a different instrument. Therefore, for the first time PyMS could be used to acquire spectra which could usefully be compared to those previously collected and held in a data-base, irresp. of the mass spectrometer used. The examples reported are for the quant. assessment of the amount of lysozyme in a binary mixture with glycogen and the rapid identification down to the species level of bacteria belonging to the genus Eubacterium. This approach is not limited solely to pyrolysis mass spectrometry but is generally applicable to any anal. tool which is prone to deterioration in calibration transfer, such as IR, ESR, NMR and other vibrational spectroscopies, gas and liquid chromatog., as well as other types of mass spectrometry.

L4 ANSWER 2 OF 4 CA COPYRIGHT 2004 ACS on STN
AB Curie-point pyrolysis mass spectrometry is a rapid, high-resolution technique which has enjoyed historical success in the operational fingerprinting and classification of microbial and other biol. systems. More recently we have exploited the anal. power of this technique together with supervised learning, based on artificial neural networks and cognate chemometric methods, for the accurate and quant. anal. of complex biol. materials, including microorganisms, fermentor broths and agricultural products. When suitable stds. are available, supervised learning is much more powerful than in unsupervised learning for the chemometric anal. of multivariate spectroscopic data. Similar neural network methods may also be used to correct for mass spectral **drift.**

L4 ANSWER 3 OF 4 CA COPYRIGHT 2004 ACS on STN
AB A method and apparatus are disclosed for analyzing a sample in which a neural network is trained to correct for measurement **drift** of a given anal. instrument (e.g., a mass spectrometer). The training is done by using first and second sets of data obtained by the instrument from samples of known compns. at initial and subsequent instants of time, resp. The trained network is used to transform data, obtained by the instrument from a sample of unknown composition at said subsequent instant of time, to an estimate of the data which would have been obtained by the instrument from that sample at the initial instant of time. The transformed data then are analyzed to analyze the sample of unknown composition Examples are given of the use of pyrolysis mass spectrometry for the determination of lysozyme and glycogen in mixture, ampicillin in Escherichia coli, Staphylococcus aureus in mixts. with Escherichia coli, and identification of human isolates of Propionibacterium acnes.

L4 ANSWER 4 OF 4 CA COPYRIGHT 2004 ACS on STN
AB For pyrolysis mass spectrometry (PyMS) to be used for the routine identification of microorganisms, for quantifying determinands in biol. and biotechnol. systems, and in the production of useful mass spectral libraries, it is paramount that newly acquired spectra be compared to those previously collected. Neural network and other multivariate

calibration models have been used to relate mass spectra to the biol. features of interest. As commonly observed, however, mass spectral fingerprints showed a lack of long-term reproducibility due to instrumental **drift** in the mass spectrometer; when identical materials were analyzed by PyMS at dates from 4 to 20 mo apart, neural network models produced at earlier times could not be used to give accurate ests. of determinand concns. or bacterial identities. Neural networks, however, can be used to correct for pyrolysis mass spectrometer instrumental **drift** itself, so that neural network or other multivariate calibration models created using previously collected data can be used to give accurate ests. of determinand concentration or the nature of bacteria (or, indeed, other materials) from newly acquired pyrolysis mass spectra. This approach is not limited solely to pyrolysis mass spectrometry but is generally applicable to any anal. tool which is prone to instrumental **drift**, such as IR, ESR, NMR and other spectroscopies, and gas and liquid chromatog., as well as other types of mass spectrometry.

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=>
=> e wilkes j/au
E1          2     WILKES IAN PETER/AU
E2          1     WILKES INGO/AU
E3         34 --> WILKES J/AU
E4          4     WILKES J B/AU
E5          3     WILKES J D/AU
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E8         25     WILKES J G/AU
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E12         1     WILKES J P/AU

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E24         3     WILKES JILLIAN/AU

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E36         1     WILKES JOHN STEPHEN/AU

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E38         2     WILKES JOHNSTON JILLIAN/AU
E39         2     WILKES JON/AU
E40        27     WILKES JON G/AU
E41         1     WILKES JON GARDNER/AU
E42         1     WILKES JONATHAN/AU
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43          6     WILKES JONATHAN M/AU
44          1     WILKES JULIE/AU
45          2     WILKES K/AU
46          6     WILKES K E/AU
47          1     WILKES K TREVOR/AU
48          1     WILKES KARL A/AU

> s e39-e41
            2 "WILKES JON"/AU
           27 "WILKES JON G"/AU
            1 "WILKES JON GARDNER"/AU
L5         30 ("WILKES JON"/AU OR "WILKES JON G"/AU OR "WILKES JON GARDNER"/AU
              )

> d ti 1-30

L5   ANSWER 1 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Predicting toxic equivalence factors from 13C nuclear magnetic resonance
     spectra for dioxins, furans, and polychlorinated biphenyls using linear
     and nonlinear pattern recognition methods

L5   ANSWER 2 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Using Simulated 2D 13C NMR Nearest Neighbor Connectivity Spectral Data
     Patterns to Model a Diverse Set of Estrogens

L5   ANSWER 3 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Carbon-13 COSY NMR data for quantitative structure-activity relationships
     and quantitative molecular structure-property relationships of
     biomolecules

L5   ANSWER 4 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Combining NMR spectral and structural data to form models of
     polychlorinated dibenzodioxins, dibenzofurans, and biphenyls binding to
     the AhR

L5   ANSWER 5 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   The use of carbon thirteen nuclear magnetic resonance spectra to predict
     dioxin and furan binding affinities to the aryl hydrocarbon receptor

L5   ANSWER 6 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Chemistry in aldol complexes of metal dications: dehydration of the
     bisligand species

L5   ANSWER 7 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Comparative structural connectivity spectra analysis (CoSCoSA) models of
     steroids binding to the aromatase enzyme

L5   ANSWER 8 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Defining and using microbial spectral databases

L5   ANSWER 9 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Microbial identification databases

L5   ANSWER 10 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Comparative structural connectivity spectra analysis (CoSCoSA) models of
     steroid binding to the corticosteroid binding globulin

L5   ANSWER 11 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Fragmentation Chemistry of DMSO Complexes of Metal Dications

L5   ANSWER 12 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Fragmentation and charge transfer in gas-phase complexes of divalent metal
     ions with acetonitrile

L5   ANSWER 13 OF 30  CA  COPYRIGHT 2004 ACS on STN
TI   Prediction of toxic equivalency factors for dioxins, furans and PCBs using
     artificial neural networks

L5   ANSWER 14 OF 30  CA  COPYRIGHT 2004 ACS on STN
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TI Developing 13C NMR quantitative spectrometric data-activity relationship (QSDAR) models of steroid binding to the corticosteroid binding globulin

L5 ANSWER 15 OF 30 CA COPYRIGHT 2004 ACS on STN
TI 13C NMR Quantitative Spectrometric Data-Activity Relationship (QSDAR) Models of Steroids Binding the Aromatase Enzyme

L5 ANSWER 16 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Models of Polychlorinated Dibenzodioxins, Dibenzofurans, and Biphenyls Binding Affinity to the Aryl Hydrocarbon Receptor Developed Using 13C NMR Data

L5 ANSWER 17 OF 30 CA COPYRIGHT 2004 ACS on STN
TI 13C NMR and Electron Ionization Mass Spectrometric Data-Activity Relationship Model of Estrogen Receptor Binding

L5 ANSWER 18 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Use of 13C NMR Spectrometric Data To Produce a Predictive Model of Estrogen Receptor Binding Activity

L5 ANSWER 19 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Electrospray mass spectrometry for mycotoxin detection and purity analysis

L5 ANSWER 20 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Producing 13C NMR, Infrared Absorption, and Electron Ionization Mass Spectrometric Data Models of the Monodechlorination of Chlorobenzenes, Chlorophenols, and Chloroanilines

L5 ANSWER 21 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Food quality indicator device to detect volatile amines

L5 ANSWER 22 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Sample preparation and high-resolution separation of mycotoxins possessing carboxyl groups

L5 ANSWER 23 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Long-term occurrence of Trypanosoma congolense resistance to diminazene, isometamidium and homidium in cattle at Ghibe, Ethiopia

L5 ANSWER 24 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Determination of underivatized fumonisin B1 and related compounds by HPLC

L5 ANSWER 25 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Multiresidue analysis of pesticides by electrospray LC-MS and LC-MS-MS

L5 ANSWER 26 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Diffusion based solvent removal interface for coupling liquid and supercritical fluid chromatography to gas chromatographic detectors

L5 ANSWER 27 OF 30 CA COPYRIGHT 2004 ACS on STN
TI AC corona-discharge aerosol-neutralization device adapted to liquid chromatography/particle beam/mass spectrometry

L5 ANSWER 28 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Particle size distribution is not the major factor explaining variable analyte transmission efficiency in liquid chromatography/particle beam/mass spectrometry

L5 ANSWER 29 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Determination of fumonisins B1, B2, B3 and B4 by high-performance liquid chromatography with evaporative light-scattering detection

L5 ANSWER 30 OF 30 CA COPYRIGHT 2004 ACS on STN
TI Application of the particle beam interface to high-performance liquid chromatography-thermal energy analysis and electron impact mass spectrometry for detection of non-volatile N-nitrosamines

=> s drift and 15

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        34318 DRIFT
L6          1 DRIFT AND L5

=> d

L6   ANSWER 1 OF 1  CA  COPYRIGHT 2004 ACS on STN
AN   137:228971  CA
TI   Microbial identification databases
IN   Wilkes, Jon G.; Rafii, Fatemeh; Glover, Katherine L.; Holcomb,
     Manuel; Cao, Xiaoxi; Sutherland, John B.
PA   The Government of the United States of America, USA
SO   U.S. Pat. Appl. Publ., 41 pp.
     CODEN: USXXCO
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
PI   US 2002138210        A1    20020926    US 2001-975530          20011010
PRAI US 2000-239549P      P     20001010


=> s identification and drift
       273269 IDENTIFICATION
        34318 DRIFT
L7        528 IDENTIFICATION AND DRIFT

=> d ti 1-10

L7   ANSWER 1 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Implications of molecular genotyping of Helicobacter pylori isolates from
     different human populations by genomic fingerprinting of enterobacterial
     repetitive intergenic consensus regions for strain identification
     and geographic evolution

L7   ANSWER 2 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Apparatus and method for focusing and selecting ions and charged particles
     at or near atmospheric pressure

L7   ANSWER 3 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Development of a Plutonium Ceramic Target for the MASHA Separator

L7   ANSWER 4 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Electrospray Ionization Ion Mobility Spectrometry of Amino Acids: Ion
     Mobilities and a Mass-Mobility Correlation

L7   ANSWER 5 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Λ production at high rapidity in d + Au collisions at √sNN =
     200 GeV

L7   ANSWER 6 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Improved identification of conjugated linoleic acid isomers
     using silver-ion HPLC separations

L7   ANSWER 7 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Basic instrumentation for Hall A at Jefferson Lab

L7   ANSWER 8 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Temperature-modulated gas sensors: selection of modulating frequencies
     through noise methods

L7   ANSWER 9 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   Status of design and construction of the Transition Radiation Tracker
     (TRT) for the ATLAS experiment at the LHC

L7   ANSWER 10 OF 528  CA  COPYRIGHT 2004 ACS on STN
TI   A straw drift chamber spectrometer for studies of rare kaon
     decays
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=> s sample drift
SAMPLE IS IGNORED AS A SCOPE FOR THIS SEARCH
L8        34318 DRIFT

=> d l7 ab

L7   ANSWER 1 OF 528  CA  COPYRIGHT 2004 ACS on STN
AB   Biogeog. partitioning of the genome is typical of the gastric pathogen
     Helicobacter pylori.  Such population-specific evolution could serve as a
     model for understanding host-pathogen interaction and the impact of
     genetic drift and recombination on insular populations.  With a
     total of 320 isolates from six geog. regions (Japan, India, England,
     Spain, Ireland, Africa, and Peru) analyzed by enterobacterial repetitive
     intergenic consensus (ERIC)-based genotyping, we examined genetic affinities
     among various H. pylori populations in the world.  Several strain-specific
     and region-specific differences were observed by ERIC-based typing.
     Polymorphic ERIC patterns indicated that the ERIC sequences are in fact
     dispersed in the H. pylori chromosome at different locations separated by
     various distances.  Phylogenetic anal. of 61 representative isolates
     revealed three distinct genetic clusters populated by isolates with shared
     ERIC types independent of the cag right-junction motif type and vacA
     allele status.  Among the notable genetic relationships were the genotypic
     similarities between Irish and Japanese and between Peruvian and Japanese
     isolates.  Insular genotypic characteristics of Irish isolates amid
     genetic similarity to East Asian, as well as North European, strains have
     been once again proved in this study.  Peruvian genotypes were more
     similar to those of Japanese isolates than to those of Iberian or European
     isolates.  Given the current debate on the origin and age of present-day
     H. pylori, this is a significant finding that supports the possibility of
     ancient colonization of Amerindians with East Asian strains.  Genotypic
     data presented here will be addnl. helpful in realizing the importance of
     H. pylori geog. genomics in the development of gastro-duodenal pathol.


=> s mass spect? and l8
        799626 MASS
       2316030 SPECT?
        260887 MASS SPECT?
                 (MASS(W)SPECT?)
L9        1126 MASS SPECT? AND L8

=> d ti 1-10

L9   ANSWER 1 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Resolution equations for high-field ion mobility

L9   ANSWER 2 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Nanoflow LC/IMS-MS and LC/IMS-CID/MS of protein mixtures

L9   ANSWER 3 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Development of Ion Drift-Chemical Ionization Mass
     Spectrometry

L9   ANSWER 4 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Construction and evaluation of polar-angle-resolved miniature
     time-of-flight ion mass spectrometer, and its
     application for electron-ion coincidence spectroscopy

L9   ANSWER 5 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Electron attachment to and anion reactions with SF5Cl: electron-swarm and
     selected ion flow tube studies

L9   ANSWER 6 OF 1126  CA  COPYRIGHT 2004 ACS on STN
TI   Peak capacity of ion mobility mass spectrometry: the
     utility of varying drift gas polarizability for the separation
     of tryptic peptides

L9   ANSWER 7 OF 1126  CA  COPYRIGHT 2004 ACS on STN
```

TI Soybean foliage residues of dicamba and 2,4-D and correlation to application rates and yield

L9 ANSWER 8 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI In situ **mass spectrometry** in a 10 Torr W chemical vapor deposition process for film thickness metrology and real-time advanced process control

L9 ANSWER 9 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI **Mass spectrometers**

L9 ANSWER 10 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Efficient direct current collision and reaction cell

=> d ti 11-20

L9 ANSWER 11 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Apparatus and method for focusing and selecting ions and charged particles at or near atmospheric pressure

L9 ANSWER 12 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Determination of thorium and uranium in Chinese foods by inductively coupled plasma **mass spectrometry**

L9 ANSWER 13 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Method and apparatus for efficient transfer of ions into a **mass spectrometer**

L9 ANSWER 14 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Time-of-flight **mass spectrometer**

L9 ANSWER 15 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Electrospray Ionization Ion Mobility Spectrometry of Amino Acids: Ion Mobilities and a Mass-Mobility Correlation

L9 ANSWER 16 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Multidynamic isotope ratio analysis using MC-ICP-MS and the causes of secular **drift** in Hf, Nd and Pb isotope ratios

L9 ANSWER 17 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI CeO2 catalysed soot oxidation. The role of active oxygen to accelerate the oxidation conversion

L9 ANSWER 18 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Dissociation pathways of protonated water clusters

L9 ANSWER 19 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Demonstration of Proton-Transfer Reaction Time-of-Flight **Mass Spectrometry** for Real-Time Analysis of Trace Volatile Organic Compounds

L9 ANSWER 20 OF 1126 CA COPYRIGHT 2004 ACS on STN
TI Compositional analysis of isobutylene/p-methylstyrene copolymers by matrix-assisted laser desorption/ionization **mass spectrometry**

=> s fingerprint and l9
6620 FINGERPRINT
L10 2 FINGERPRINT AND L9

=> d ti 1-2

L10 ANSWER 1 OF 2 CA COPYRIGHT 2004 ACS on STN
TI Microbial identification databases

L10 ANSWER 2 OF 2 CA COPYRIGHT 2004 ACS on STN
TI Gas Sensors Arrays ('Electronic Noses'): a study about the speed/accuracy

ratio

=> d 1 ab

L10 ANSWER 1 OF 2 CA COPYRIGHT 2004 ACS on STN
AB Methods of compensating for **drift** in **fingerprint** spectra of microorganisms caused by changes in their environment are disclosed. These methods of compensating for **drift** permit identification of microorganisms from their **fingerprint** spectra regardless of the environment from which the microorganisms are obtained. Furthermore, the disclosed methods may be used to construct coherent databases of **fingerprint** spectra that may be expanded even though the standard database conditions are no longer exptl. achievable. In particular embodiments, methods of compensating for **drift** in pyrolysis **mass spectra**, constructing coherent pyrolysis **mass spectral** databases, and identifying bacteria from their pyrolysis **mass spectra** are disclosed.

=> d

L10 ANSWER 1 OF 2 CA COPYRIGHT 2004 ACS on STN
AN 137:228971 CA
TI Microbial identification databases
IN Wilkes, Jon G.; Rafii, Fatemeh; Glover, Katherine L.; Holcomb, Manuel; Cao, Xiaoxi; Sutherland, John B.
PA The Government of the United States of America, USA
SO U.S. Pat. Appl. Publ., 41 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002138210	A1	20020926	US 2001-975530	20011010
PRAI	US 2000-239549P	P	20001010		

=> s specimen
L11 91655 SPECIMEN

=> d his

(FILE 'HOME' ENTERED AT 14:52:08 ON 15 NOV 2004)

FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004
E GOODACRE/AU
E GOODACRE ROYSTON/AU
L1 22 S E3
L2 0 S L1 AND DRIFT

FILE 'CA' ENTERED AT 14:54:30 ON 15 NOV 2004
E GOODACRE R/AU
L3 86 S E6
L4 4 S DRIFT AND L3
E WILKES J/AU
L5 30 S E39-E41
L6 1 S DRIFT AND L5
L7 528 S IDENTIFICATION AND DRIFT
L8 34318 S SAMPLE DRIFT
L9 1126 S MASS SPECT? AND L8
L10 2 S FINGERPRINT AND L9
L11 91655 S SPECIMEN

=> s l11 and l8
L12 213 L11 AND L8

> d ti 1-10

L2 ANSWER 1 OF 213 CA COPYRIGHT 2004 ACS on STN
Development of coincidence transmission electron microscope. III. Incorporation with γ-type imaging energy filter

L2 ANSWER 2 OF 213 CA COPYRIGHT 2004 ACS on STN
Improvesments in dimensional stability and lightfastness of wood by butyrylation using microwave heating

L2 ANSWER 3 OF 213 CA COPYRIGHT 2004 ACS on STN
Analytical electron microscopy of InP/(In, Ga)As heterogeneous structures

L2 ANSWER 4 OF 213 CA COPYRIGHT 2004 ACS on STN
The use of environmental scanning electron microscopy for imaging wet and insulating materials

L2 ANSWER 5 OF 213 CA COPYRIGHT 2004 ACS on STN
Investigation of the change in the **DRIFT** spectra of light-irradiated wood with heat treatment

L2 ANSWER 6 OF 213 CA COPYRIGHT 2004 ACS on STN
Characteristics of carrier mobility in polyaniline

L2 ANSWER 7 OF 213 CA COPYRIGHT 2004 ACS on STN
Surface Modification of Colloidal Silica by Sulfonation Route for Super-Hydrophilicity

L2 ANSWER 8 OF 213 CA COPYRIGHT 2004 ACS on STN
Characterization of metal-ceramic interfaces using low voltage x-ray microanalysis in a field emission scanning electron microscope

L2 ANSWER 9 OF 213 CA COPYRIGHT 2004 ACS on STN
Drift in the hypervariable region of the hepatitis C virus during 27 years in two patients

L2 ANSWER 10 OF 213 CA COPYRIGHT 2004 ACS on STN
Electron **drift** mobility in polystyrene doped with bispyrazolopyridine derivatives

> d ti 11-20

L2 ANSWER 11 OF 213 CA COPYRIGHT 2004 ACS on STN
A new method for the determination of the wave aberration function for high resolution TEM 1. Measurement of the symmetric aberrations

L2 ANSWER 12 OF 213 CA COPYRIGHT 2004 ACS on STN
A **specimen-drift**-free EDX mapping system in a STEM for observing two-dimensional profiles of low dose elements in fine semiconductor devices

L2 ANSWER 13 OF 213 CA COPYRIGHT 2004 ACS on STN
Automated Data Collection with a Tecnai 12 Electron Microscope: Applications for Molecular Imaging by Cryomicroscopy

L2 ANSWER 14 OF 213 CA COPYRIGHT 2004 ACS on STN
Automated analysis of submicron particles by CCSEM / EDXS - where are the limits?

L2 ANSWER 15 OF 213 CA COPYRIGHT 2004 ACS on STN
Automated analysis of submicron particles by computer-controlled scanning electron microscopy

L2 ANSWER 16 OF 213 CA COPYRIGHT 2004 ACS on STN
Scanning probe microscope, method for measuring band structure of substance by using the microscope, and microscopic spectroscopy

L2 ANSWER 17 OF 213 CA COPYRIGHT 2004 ACS on STN

I Step bunching, step wandering and faceting. Self-organization at Si surfaces

12 ANSWER 18 OF 213 CA COPYRIGHT 2004 ACS on STN
I Analysis of nanoscale multilayers by EDXS and EELS in the STEM

12 ANSWER 19 OF 213 CA COPYRIGHT 2004 ACS on STN
I The adsorption and curing behaviors of the epoxy/amidoamine system in the presence of metal oxides

12 ANSWER 20 OF 213 CA COPYRIGHT 2004 ACS on STN
I A novel multicell silicon **drift** detector module for x-ray spectroscopy and imaging applications

> d ab 12

12 ANSWER 12 OF 213 CA COPYRIGHT 2004 ACS on STN
B We developed a **specimen**-**drift**-free energy-dispersive X-ray (EDX) mapping system in a scanning transmission electron microscope (STEM) to improve the sensitivity and spatial resolution of EDX elemental mapping images. The amount of **specimen drift** was analyzed from two STEM images before and after **specimen drift** by using the phase-correlation method, and was compensated for with an image-shift deflector of the STEM by the displacement of the scanning electron beam. We applied this system to observe the two-dimensional distribution of low dose arsenic in silicon semiconductor devices. The sensitivity of the elemental mapping was improved to several tenths atomic % for arsenic atoms while maintaining a spatial resolution of 2 nm.

> d l12 and fingerprint?
AND' IS NOT A VALID FORMAT FOR FILE 'CA'
FINGERPRINT?' IS NOT A VALID FORMAT FOR FILE 'CA'

he following are valid formats:

BS --------- GI and AB
LL --------- BIB, AB, IND, RE
PPS -------- AI, PRAI
IB --------- AN, plus Bibliographic Data and PI table (default)
AN --------- List of CA abstract numbers without answer numbers
BIB -------- AN, plus Compressed Bibliographic Data
ALL -------- ALL, delimited (end of each field identified)
MAX -------- MAX, delimited for post-processing
AM --------- AN, PI and PRAI in table, plus Patent Family data
BIB -------- AN, BIB, plus Patent FAM
ND --------- Indexing data
PC --------- International Patent Classifications
AX --------- ALL, plus Patent FAM, RE
ATS -------- PI, SO
AM --------- CC, SX, TI, ST, IT
CAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
TD --------- BIB, IPC, and NCL

ABS -------- ABS, indented with text labels
ALL -------- ALL, indented with text labels
BIB -------- BIB, indented with text labels
MAX -------- MAX, indented with text labels
STD -------- STD, indented with text labels

BIB -------- AN, plus Bibliographic Data (original)
IBIB ------- OBIB, indented with text labels

BIB -------- BIB, no citations
IBIB ------- IBIB, no citations

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IT --------- Fields containing hit terms
ITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
             containing hit terms
ITRN ------- HIT RN and its text modification
ITSTR ------ HIT RN, its text modification, its CA index name, and
             its structure diagram
ITSEQ ------ HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
HITSTR ----- First HIT RN, its text modification, its CA index name, and
             its structure diagram
HITSEQ ----- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
WIC -------- Hit term plus 20 words on either side
CC --------- Number of occurrence of hit term and field in which it occurs

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odes.  For a list of the display field codes, enter HELP DFIELDS at
n arrow prompt (=>).  Examples of formats include: TI; TI,AU; BIB,ST;
I,IND; TI,SO.  You may specify the format fields in any order and the
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ll of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
HITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
o view a specified Accession Number.
NTER DISPLAY FORMAT (BIB):
NTER DISPLAY FORMAT (BIB):bib

12  ANSWER 1 OF 213  CA  COPYRIGHT 2004 ACS on STN
N   141:342470  CA
I   Development of coincidence transmission electron microscope. III.
    Incorporation with γ-type imaging energy filter
J   Nishinaka, Kenichi; Taka, Shinsuke; Kimura, Yoshihide; Takai, Yoshizo
S   Department of Material and Life Science, Graduate School of Engineering,
    Osaka University, Suita, Osaka, 565-0871, Japan
O   Journal of Electron Microscopy (2004), 53(3), 217-222
    CODEN: JELJA7; ISSN: 0022-0744
B   Oxford University Press
T   Journal
A   English
E.CNT  11    THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
             ALL CITATIONS AVAILABLE IN THE RE FORMAT


> s l12 and fingerprint?
        16668 FINGERPRINT?
13          0 L12 AND FINGERPRINT?

> d his

    (FILE 'HOME' ENTERED AT 14:52:08 ON 15 NOV 2004)

    FILE 'MEDLINE' ENTERED AT 14:52:40 ON 15 NOV 2004
              E GOODACRE/AU
              E GOODACRE ROYSTON/AU
1           22 S E3
2            0 S L1 AND DRIFT

    FILE 'CA' ENTERED AT 14:54:30 ON 15 NOV 2004
              E GOODACRE R/AU
3           86 S E6
4            4 S DRIFT AND L3
              E WILKES J/AU
5           30 S E39-E41
6            1 S DRIFT AND L5
7          528 S IDENTIFICATION AND DRIFT
8        34318 S SAMPLE DRIFT
9         1126 S MASS SPECT? AND L8
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0           2 S FINGERPRINT AND L9
1       91655 S SPECIMEN
2         213 S L11 AND L8
3           0 S L12 AND FINGERPRINT?

 s drift and fingerprint? amd l11
SSING OPERATOR AMD L11
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sted terms that are not separated by a logical operator.

 s drift and fingerprint? and l11
       34318 DRIFT
       16668 FINGERPRINT?
4          0 DRIFT AND FINGERPRINT? AND L11

 s drift and fingerprint?
       34318 DRIFT
       16668 FINGERPRINT?
5         41 DRIFT AND FINGERPRINT?

 d ti 1-10

5  ANSWER 1 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Implications of molecular genotyping of Helicobacter pylori isolates from
   different human populations by genomic fingerprinting of
   enterobacterial repetitive intergenic consensus regions for strain
   identification and geographic evolution

5  ANSWER 2 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Silylation and surface properties of chemically grafted hydrophobic silica

5  ANSWER 3 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Population genetic structure of Titanotrichum oldhamii (Gesneriaceae), a
   subtropical bulbiliferous plant with mixed sexual and asexual reproduction

5  ANSWER 4 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Molecular epidemiology and diagnosis of Leishmania: what have we learnt
   from genome structure, dynamics and function?

5  ANSWER 5 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Genetic diversity of selected bacterial populations in North Carolina

5  ANSWER 6 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Microbial identification databases

5  ANSWER 7 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Nonlinear electrophoresis and focusing of macromolecules

5  ANSWER 8 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Interpretation of band differences to distinguish strains of Serratia
   marcescens by pulsed-field gel electrophoresis of XbaI DNA digests

5  ANSWER 9 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Gas Sensors Arrays ('Electronic Noses'): a study about the speed/accuracy
   ratio

5  ANSWER 10 OF 41  CA  COPYRIGHT 2004 ACS on STN
   Low RAPD polymorphism in Archangiopteris itoi, a rare and endemic fern in
   Taiwan

 d ab 8

5  ANSWER 8 OF 41  CA  COPYRIGHT 2004 ACS on STN
   The number of band differences in DNA macrorestriction profiles required to
   distinguish unrelated strains from an index strain varies in an outbreak
   with the species and restriction enzyme used.  In order to define this
   difference for epidemiol. studies of Serratia marcescens, we produced DNA
   fingerprints from 57 isolates of the organism using the
```

restriction enzyme XbaI and pulsed-field gel electrophoresis (PFGE). The isolates were selected on the basis of their epidemiol., serotype and phage-typing patterns to include 28 unrelated strains and 29 representatives from 2 distinct outbreaks. One of the outbreaks was prolonged, lasting for several years. Electrophoretic profiles consisting of 20 or more clearly resolved bands were obtained for all isolates. Twenty-six of the unrelated strains had unique profiles with over 10 band differences from all other strains, while 27 of the outbreak representatives could be assigned to the appropriate outbreak with confidence. The majority of the outbreak isolates had none or 2 band differences from the index profile, although 3 isolates differed by 5-7 bands. The 2 exceptions among the unrelated strains differed by 4 bands, and 3 phage typing reactions, and were isolated from London and Berlin 3 yr apart, while the 2 exceptions among the outbreak collection had clearly unique profiles with over 20 band differences from each other and the outbreak profiles. Cluster anal. using Dice coefficient and UPGMA gave cut-off values of 75-78% similarity overall for related isolates, while the closest similarity for unrelated strains was 70%. The results of this study together with those of the 6 previous reports of PFGE for S. marcescens (which used either enzymes XbaI or SpeI) confirm that this technique is of value for this species and that with XbaI at least, most epidemiol. related strains will only differ by 3-4 bands. However, on occasion up to 7 band differences can be found within an apparent outbreak, which may be suggestive of genetic **drift.**

> d ab 7

15 ANSWER 7 OF 41 CA COPYRIGHT 2004 ACS on STN
B Effects of nonlinear dependence **drift** velocity of (double-stranded) DNA vs. elec. field strength were investigated. In comparatively weak fields, the mol. **drift** velocity is proportional to the external elec. field, while in strong fields there is addnl. nonlinear component. This effect offers possibilities to manipulate the total **drift** velocity at will-the macromols. of different size can be made to move in opposite directions in pulsed field gel electrophoresis. A new approach for focusing DNA mols. based on nonlinear electrophoresis and geometric trapping in elec. fields is proposed. The focusing is carried out in an alternating nonuniform elec. field, created by using a wedge gel with hyperbolic boundaries. It is shown that the fractions separated in such wedge retain their rectilinear shape. Gel electrophoresis expts. supported the possibility of a pronounced nonlinear focusing of DNA mols. This nonlinear separation technique presents encouraging prospects for micromanipulating systems and also for preparative isolation of long DNA fragments and development of new separation methods for bacterial **fingerprinting.**

> d ti 11-20

15 ANSWER 11 OF 41 CA COPYRIGHT 2004 ACS on STN
I **Fingerprinting** of Helicobacter pylori strains by matrix-assisted laser desorption/ionization mass spectrometric analysis

15 ANSWER 12 OF 41 CA COPYRIGHT 2004 ACS on STN
I Variation of multilocus minisatellite DNA **fingerprints** in avian populations

15 ANSWER 13 OF 41 CA COPYRIGHT 2004 ACS on STN
I FTIR-spectroscopy in microbial and material analysis

15 ANSWER 14 OF 41 CA COPYRIGHT 2004 ACS on STN
I Development of an optimized sorbent for direct HPTLC-FTIR online coupling

15 ANSWER 15 OF 41 CA COPYRIGHT 2004 ACS on STN
I Channel plate for electrophoretic DNA sequencing

15 ANSWER 16 OF 41 CA COPYRIGHT 2004 ACS on STN
I Application of laser microprobe inductively coupled plasma mass

spectrometry for trace metal **fingerprinting** of native gold

L15 ANSWER 17 OF 41 CA COPYRIGHT 2004 ACS on STN
TI Separation of polyester oligomers by gradient high-performance liquid chromatography

L15 ANSWER 18 OF 41 CA COPYRIGHT 2004 ACS on STN
TI Mid-infrared as a new tool for detecting adulteration in fruit products

L15 ANSWER 19 OF 41 CA COPYRIGHT 2004 ACS on STN
TI Rapid analysis of multiple determinands using pyrolysis mass spectrometry and supervised learning with artificial neural networks - principles and applications

L15 ANSWER 20 OF 41 CA COPYRIGHT 2004 ACS on STN
TI FTIR spectroscopy

=> d 13,19 ab

L15 ANSWER 13 OF 41 CA COPYRIGHT 2004 ACS on STN
AB The investigation of the development and the properties of biofilms is difficult because classical microbiol. does not offer non-destructive methods other than microscopical observations. This paper discusses the use of different Fourier transform IR spectroscopy (FTIR-spectroscopy) techniques as a means to investigate microorganisms in biofilms. FTIR-spectroscopy is suitable for the identification of microorganisms and presents a new addition to taxonomic and genetic methods. The FTIR anal. of bacterial isolates provides **fingerprint** spectra, allowing the rapid characterization of microbial strains. Secondly, the FTIR-attenuated total reflection (ATR) technique can be used for the observation of biofilms forming directly on the interface of an ATR crystals such as germanium. These crystals can be coated to obtain a surface more relevant to study interfacial processes. Spectra can be acquired non-destructively, in situ and in real time. This method is suitable for fundamental biofilm research, as well as for monitoring of biofilm formation, e.g., in an ultrapure or drinking water systems. Furthermore, FTIR-ATR also allows the rapid anal. of deposits on surfaces, e.g., filtration membranes. The anal. discrimination between microorganisms, inorg. material or other foulants can be obtained. Thirdly, with the diffuse reflectance technique (**DRIFT**) it is possible to investigate reflecting surfaces like metals or very small samples. The composition of surface coatings like biomass or other surface contaminants can be detected. These different measurement techniques demonstrate that FTIR -spectroscopy is suitable for biofilm and surface anal. and can be applied in many different ways.

15 ANSWER 19 OF 41 CA COPYRIGHT 2004 ACS on STN
AB Curie-point pyrolysis mass spectrometry is a rapid, high-resolution technique which has enjoyed historical success in the operational **fingerprinting** and classification of microbial and other biol. systems. More recently we have exploited the anal. power of this technique together with supervised learning, based on artificial neural networks and cognate chemometric methods, for the accurate and quant. anal. of complex biol. materials, including microorganisms, fermentor broths and agricultural products. When suitable stds. are available, supervised learning is much more powerful than in unsupervised learning for the chemometric anal. of multivariate spectroscopic data. Similar neural network methods may also be used to correct for mass spectral **drift.**

> d 19

15 ANSWER 19 OF 41 CA COPYRIGHT 2004 ACS on STN
N 127:106297 CA
I Rapid analysis of multiple determinands using pyrolysis mass spectrometry and supervised learning with artificial neural networks - principles and applications